

Heat transport along a chain of coupled quantum harmonic oscillators

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We study the heat transport properties of a chain of coupled quantum harmonic oscillators in contact at its ends with two heat reservoirs at distinct temperatures. Our approach is based on the use of an evolution equation for the density operator which is a canonical quantization of the classical Fokker-Planck-Kramers equation. We set up the evolution equation for the covariances and obtain the stationary covariances at the stationary states from which we determine the thermal conductance in closed form when the interparticle interaction is small. The conductance is finite in the thermodynamic limit implying an infinite thermal conductivity.

Fifty years ago, Rieder, Lebowitz, and Lieb [1] introduced and exactly solved a microscopic model for thermal conduction, that consisted of a chain of coupled classic harmonic oscillators with its ends in contact with heat reservoirs at distinct temperatures. Using this model they provided a rigorous proof of the well known result that the thermal conductance, the ratio between the heat current and the temperature difference, is finite regardless of the chain length [2]. This result amounts to say that Fourier's law does not hold because the conductivity, which is the product of the conductance and the chain length, becomes infinite when the length increases without bounds. The reason for the occurrence of a finite conductance is that the excitations in ordered systems with harmonic interactions travel ballistically. To get the Fourier's law, new ingredients should be added to the harmonic model in order to transform the ballistic into a diffusive motion. Such ingredients include anharmonic potentials [3–8], self-consistent reservoirs [9–12], energy conserving noise [13–15], and others [16–20].

In the model studied by Rieder, Lebowitz, and Lieb [1], the oscillators were under the action of conservative forces except the first and the last which in addition were subject to dissipating-fluctuating forces representing the contact with heat reservoirs. They are composed by a dissipative force, proportional to the velocity, and a Gaussian white noise with zero mean and variance proportional to the temperature. The equations of motion are understood as Langevin equations, and the equation governing the time evolution of the probability density is a Fokker-Planck-Kramers (FPK) equation [21–24].

Here, we study a quantum version of the model studied by Rieder, Lebowitz, and Lieb [1]. We have exactly calculated the thermal conductance in the regime of small interparticle interaction and reached a similar result that the conductance is finite regardless of the length of the chain. However, as should be expected the conductance is not independent of temperature, as is the case of the classical version. It vanishes in the limit of zero temperature and saturates at the classical value at high temperatures. Our approach is based on a quantum version of the FPK equation coming from a canonical quantization of the ordinary FPK equation, recently introduced [25], and

differs from other approaches regarding the treatment of quantum dissipation [26–36]. These approaches include the use of quantum Langevin equations [26, 30, 31], and the use of the rotating wave approximation and Lindblad master equation to describe the contact with heat reservoirs [32, 34]. These approaches as well as ours, when applied to the harmonic chain, predict a finite conductance regardless of the chain length [26, 34]. It worth mentioning that the approach we use leads to a proper thermalization in the sense that the Gibbs equilibrium state is the stationary solution of the quantum FPK equation when the reservoirs have the same temperatures [25].

The model we consider is a chain of L particles of equal masses interacting through a harmonic potential. The quantum hamiltonian of the system is given by

$$\mathcal{H} = \frac{1}{2m} \sum_{i=1}^L p_i^2 + \frac{k_0}{2} \sum_{i=1}^L q_i^2 - k_1 \sum_{i=1}^{L-1} q_i q_{i+1}, \quad (1)$$

where m is the mass of the particles, k_0 is the spring constant and k_1 is the interparticle interacting parameter. The position q_i and momentum p_i obey the usual commutation relation, $[q_i, p_j] = i\hbar\delta_{ij}$. To describe the contact of the system with heat reservoirs we use the quantum Fokker-Planck-Kramers (FPK) equation [25] with the first particle of the chain in contact with a heat reservoir A at temperature T_A and the last with a reservoir B at temperature T_B . The quantum FPK equation reads [25]

$$i\hbar \frac{\partial \rho}{\partial t} = [\mathcal{H}, \rho] - [q_1, J_1] - [q_L, J_L], \quad (2)$$

where ρ is the density matrix, and J_1 and J_2 are given by

$$J_i = -\frac{\gamma}{2}(\rho g_i + g_i^\dagger \rho) - \frac{\gamma m}{i\hbar\beta_i}[q_i, \rho], \quad (3)$$

where γ is the dissipation parameter and $\beta_i = 1/k_B T_i$, with $T_1 = T_A$ and $T_L = T_B$. The operator g_i is given by

$$g_i = -\frac{m}{i\hbar\beta_i}(e^{\beta_i \mathcal{H}} q_i e^{-\beta_i \mathcal{H}} - q_i). \quad (4)$$

When the temperatures are the same, the Gibbs density $\rho_0 = (1/Z)e^{-\beta\mathcal{H}}$ is the stationary equilibrium solution of the quantum FPK equation (2) because it makes each one of the J_i to vanish and $[\mathcal{H}, \rho_0] = 0$.

The operator g_i can be written in a form involving nested commutators

$$g_i = p_i + \frac{\beta_i}{2!}[\mathcal{H}, p_i] + \frac{\beta_i^2}{3!}[\mathcal{H}, [\mathcal{H}, p_i]] + \frac{\beta_i^3}{4!}[\mathcal{H}, [\mathcal{H}, [\mathcal{H}, p_i]]] + \dots \quad (5)$$

Taking into account the bilinear form of \mathcal{H} and that the coordinates are not coupled to the momenta, we notice that the odd terms in this expansion are linear combinations of the momenta only, and that the even terms are linear combinations of the coordinates only. From these properties, it follows that g_i is a linear combination of the positions and momenta,

$$g_i = \sum_{j=1}^L (a_{ij}p_j + ib_{ij}q_j), \quad (6)$$

where the coefficients a_{ij} and b_{ij} depend on the temperature T_i and on the parameters of the Hamiltonian. In addition, using the fact that the odd terms are Hermitian and that the even terms are anti-Hermitian it follows that the coefficient of p_j is real and the coefficient of q_j is pure imaginary so that a_{ij} and b_{ij} are real.

Next, we wish to write down evolution equations for the averages of quantities of interest in our analysis. The evolution equation for a certain average $\langle f \rangle = \text{Tr}\{f\rho\}$ of an operator f can be obtained from the quantum FPK equation (2) and it is given by

$$i\hbar \frac{d}{dt} \langle f \rangle = \langle [f, H] \rangle - \text{Tr}[f, q_1]J_1 - \text{Tr}[f, q_L]J_L, \quad (7)$$

$$\text{Tr}[f, q_i]J_i = -\frac{\gamma}{2} \langle g_i[f, q_i] \rangle - \frac{\gamma}{2} \langle [f, q_i]g_i^\dagger \rangle - \frac{\gamma m}{i\hbar\beta_i} \langle [[f, q_i], q_i] \rangle. \quad (8)$$

From this formula we get at once

$$\frac{d}{dt} \langle \mathcal{H} \rangle = \Phi_1 + \Phi_L \quad (9)$$

where $\Phi_i = (1/m)\text{Tr}p_iJ_i$ is the energy flux from reservoir i to the chain.

Using formula (7) we get the evolution equation for the correlations among the coordinates and momenta, $x_{ij} = \langle q_i q_j \rangle$, $y_{ij} = \langle p_i p_j \rangle$, and $z_{ij} = \langle q_i p_j \rangle$,

$$\frac{d}{dt} x_{ij} = \frac{1}{m} (z_{ij} + \tilde{z}_{ij}), \quad (10)$$

$$\frac{d}{dt} z_{ij} = -\sum_{k=1}^L x_{ik} G_{kj} + \frac{1}{m} y_{ij} - \frac{\gamma}{2} \sum_{k=1}^L a_{jk} (\tilde{z}_{ki} + z_{ik}), \quad (11)$$

$$\begin{aligned} \frac{d}{dt} y_{ij} = & -\sum_{k=1}^L (G_{ik} z_{kj} + \tilde{z}_{ik} G_{kj}) + 2\gamma m \delta_{ij} \left(\frac{\delta_{j1}}{\beta_1} + \frac{\delta_{jL}}{\beta_L} \right) \\ & - \gamma \sum_{k=1}^L (a_{jk} y_{ki} + a_{ik} y_{kj}) + \frac{\gamma \hbar}{2} (b_{ji} + b_{ij}), \end{aligned} \quad (12)$$

where $\tilde{z}_{ij} = \langle p_i q_j \rangle$, and G_{ij} are the elements of a tridiagonal matrix G , with $G_{ii} = k_0$, and $G_{i,i+1} = G_{i+1,i} = -k_1$. In these equations, we are setting the coefficients a_{ij} and b_{ij} to vanish unless $i = 1$ or $i = L$. We see that equations (10), (11), and (12) make up a closed set of equations for the correlations x_{ij} , y_{ij} , and z_{ij} by recognizing that $\tilde{z}_{ji} = z_{ij} - i\hbar\delta_{ij}$.

In the stationary state, $\Phi_L = -\Phi_1$ and $\Phi = \Phi_L$ may thus be understood as the heat flux from reservoir B to reservoir A through the chain. Using equations (10) and (12), we can show that $z_{21} = z_{32} = \dots = z_{L,L-1}$, that $z_{ji} = -z_{ij}$, and that $\Phi = (k_1/m)z_{i+1,i}$, a relation that will be used to determine the conductance.

To simplify the evolution equations, we will subtract the equilibrium solution, which we denote by x_{ij}^e , y_{ij}^e , and z_{ij}^e . By equilibrium solution we mean the stationary solution of (10), (11), and (12) for the case when both temperatures of the reservoirs are the same and equal to $T = (T_1 + T_L)/2$. In equilibrium $z_{ij}^e = \tilde{z}_{ij}^e = 0$ if $i \neq j$ and $z_{ii}^e = -\tilde{z}_{ii}^e = i\hbar/2$. The correlations x_{ij}^e and y_{ij}^e are given by

$$\sum_{k=1}^L x_{ik}^e G_{kj} = \frac{1}{m} y_{ij}^e, \quad (13)$$

$$\sum_{k=1}^L (A_{jk} y_{ki}^e + A_{ik} y_{kj}^e) = \frac{\hbar}{2} (B_{ji} + B_{ij}) + \frac{2m}{\beta} \delta_{ij} (\delta_{j1} + \delta_{jL}), \quad (14)$$

where $\beta = 1/k_B T$, and A_{ik} and B_{ik} are the values of a_{ij} and b_{ij} that one obtains by replacing both β_1 and β_L by β . The quantities A_{ij} and B_{ij} are nonzero only when $i = 1$ or $i = L$ in which case they hold the property $A_{Lj} = A_{1,L+1-j}$ and $B_{Lj} = B_{1,L+1-j}$.

We define the deviations $X_{ij} \Delta T = x_{ij} - x_{ij}^e$, $Y_{ij} \Delta T = y_{ij} - y_{ij}^e$, $Z_{ij} \Delta T = z_{ij} - z_{ij}^e$, and $\tilde{Z}_{ij} \Delta T = \tilde{z}_{ij} - \tilde{z}_{ij}^e$ from the equilibrium solution, where $\Delta T = T_L - T_1$. We remark that $\tilde{Z}_{ij} = Z_{ji}$. We wish, in the following, to write down evolution equations for the variables X_{ij} , Y_{ij} , and Z_{ij} for small values of ΔT . In this regime the evolution equation reads

$$\frac{d}{dt} X_{ij} = \frac{1}{m} (Z_{ij} + \tilde{Z}_{ij}), \quad (15)$$

$$\frac{d}{dt} Z_{ij} = -\sum_{k=1}^L X_{ik} G_{kj} + \frac{1}{m} Y_{ij} - \frac{\gamma}{2} \sum_{k=1}^L A_{jk} (\tilde{Z}_{ki} + Z_{ik}), \quad (16)$$

$$\begin{aligned} \frac{d}{dt}Y_{ij} = & -\sum_{k=1}^L (G_{ik}Z_{kj} + \tilde{Z}_{ik}G_{kj}) + \gamma m k_B \delta_{ij} (-\delta_{j1} + \delta_{jL}) \\ & - \gamma \sum_{k=1}^L (A_{jk}Y_{ki} + A_{ik}Y_{kj}) - \gamma(C_{ji} + C_{ij}), \end{aligned} \quad (17)$$

where

$$C_{ij}\Delta T = \sum_{k=1}^L (a_{ik} - A_{ik})y_{kj}^e - \frac{\hbar}{2}(b_{ij} - B_{ij}), \quad (18)$$

The quantities C_{ij} are nonzero only when $i = 1$ or $i = L$ in which case they hold the property $C_{Lj} = -C_{1,L+1-j}$.

These equations are written in matrix form as

$$\frac{d}{dt}X = \frac{1}{m}(Z + Z^\dagger), \quad (19)$$

$$\frac{d}{dt}Z = -XG + \frac{1}{m}Y - \gamma ZA^\dagger, \quad (20)$$

$$\frac{d}{dt}Y = -(GZ + Z^\dagger G) + \gamma D - (YA^\dagger + AY) - \gamma(C^\dagger + C), \quad (21)$$

where the matrix D has only two nonzero elements, which are $D_{11} = -mk_B$ and $D_{LL} = mk_B$. It should be noted that all the entries of X , Y , and Z are real and that X and Y are symmetric matrices. All entries of matrices G , A and C are also real and G is symmetric. The matrices A and C have nonzero values only on the first and the last row.

In the stationary state we are left with the equations

$$Z = -Z^\dagger, \quad (22)$$

$$Y = m(XG + \gamma ZA^\dagger), \quad (23)$$

$$Y = m(GX - \gamma AZ), \quad (24)$$

$$\gamma D - \gamma(YA^\dagger + AY) - \gamma(C + C^\dagger) = GZ - ZG. \quad (25)$$

In the classical limit, C vanishes and A becomes a matrix whose only nonzero entries are $A_{11} = 1$ and $A_{LL} = 1$, and we recover the equations obtained by Rieder, Lebowitz, and Lieb [1].

Our next step is to seek the solution of equations (22), (23), (24), and (25). To this end we follow the reasoning put forward by Rieder, Lebowitz, and Lieb [1]. We start by observing that the left-hand side of equation (25) is a bordered matrix, that is, a matrix whose nonvanishing entries are found only in the first and last rows and columns. Therefore, the right-hand side $GZ - ZG$ should also be bordered. Using the definition of G and the relation $Z_{ji} = -Z_{ij}$, that comes from (22) and the property

that Z_{ij} is real, it follows that Z is an antisymmetric Toeplitz matrix, that is, a matrix of the type

$$Z_{ij} = \begin{cases} \varphi_{j-i}, & i < j, \\ 0, & i = j, \\ -\varphi_{i-j}, & i > j. \end{cases} \quad (26)$$

From equations (23) and (24), we get the following relation between X and Z ,

$$XG - GX = -\gamma(AZ + ZA^\dagger). \quad (27)$$

The right-hand side of this equation is again a bordered matrix and so is the matrix $XG - GX$. Since X is required to be symmetric, a solution for X is an antisymmetric Hankel matrix, that is, a matrix of the following form

$$X_{ij} = \begin{cases} \psi_{i+j-1}, & i + j < L + 1, \\ 0, & i + j = L + 1, \\ -\psi_{2L+1-i-j}, & i + j > L + 1. \end{cases} \quad (28)$$

Replacing (28) into (27), we find ψ_i in terms of φ_i

$$\frac{k_1}{\gamma}\psi_\ell = -\sum_{j=1}^L \eta_{\ell,j-1} A_j \varphi_{|\ell-j+1|}, \quad (29)$$

$1 \leq \ell < L$, where A_j stands for A_{1j} and $\eta_{\ell,j} = -1, 0, 1$ according to whether $j < \ell$, $j = \ell$, $j > \ell$, respectively.

From equations (23) and (24), it is straightforward to show that Y is also an antisymmetric Hankel matrix, that is, a matrix of the following form

$$Y_{ij} = \begin{cases} \theta_{i+j-1}, & i + j < L + 1, \\ 0, & i + j = L + 1, \\ -\theta_{2L+1-i-j}, & i + j > L + 1, \end{cases} \quad (30)$$

and that θ_ℓ is related to ψ_ℓ by

$$\theta_\ell = m(k_0 \psi_\ell - k_1 \psi_{\ell+1} - k_1 \psi_{\ell-1}), \quad (31)$$

$1 \leq \ell < L$, where $\psi_0 = 0$ and $\psi_L = 0$.

Since ψ_ℓ is related to φ_ℓ by expression (29), then equation (31) gives θ_ℓ in terms of φ_ℓ . To get a closed equation for φ_ℓ we use equation (25) to obtain another relation between φ_ℓ and θ_ℓ , namely

$$\frac{k_1}{\gamma}\varphi_\ell = -\frac{m}{2}k_B\delta_{\ell 1} - \sum_{j=1}^L \eta_{\ell,L+1-j} A_j \theta_{L-|L+1-\ell-j|} - C_\ell, \quad (32)$$

$1 \leq \ell < L$, where C_ℓ stands for $C_{1\ell}$. Therefore, equations (29), (31), and (32) constitute the desired closed equations for the variables φ_ℓ . To solve them we need to know A_ℓ and B_ℓ because C_ℓ is related to these quantities by

$$C_\ell = -\frac{1}{2} \sum_{k=1}^L \frac{dA_k}{dT} y_{k\ell}^e + \frac{\hbar}{4} \frac{dB_\ell}{dT}, \quad (33)$$

which follows from (18), where B_ℓ stands for $B_{1\ell}$. We recall that A_ℓ and B_ℓ depend on T and are the values of $a_{1\ell}$ and $b_{1\ell}$ obtaining by setting T_1 equal to T .

Explicit solutions of equations (29), (31), and (32) are very cumbersome to find, but closed solutions can be found when the interparticle interaction is small. Thus, from now on we will confine ourselves to the case where the interparticle interacting parameter k_1 is small. To this end, we first notice that the quantities A_ℓ and B_ℓ are of the order $k_1^{\ell-1}$ and so is C_ℓ , a result that follows from expansion (5). Thus, from equations (29), (31), and (32) it follows that φ_ℓ , θ_ℓ , and ψ_ℓ are of order greater or equal k_1 , except θ_1 and ψ_1 , which are

$$\theta_1 = -\frac{1}{2A_1}(mk_B + 2C_1), \quad \psi_1 = \frac{1}{mk_0}\theta_1 \quad (34)$$

Using equation (29), we see that φ_1 is of the order k_1 and given by

$$\varphi_1 = \frac{k_1}{\gamma A_1}\psi_1. \quad (35)$$

The conductance K is defined as the ratio $K = \Phi/\Delta T$ in the limit $\Delta T \rightarrow 0$. To determine K , we recall that, in the stationary state, the heat flux $\Phi = (k_1/m)z_{i+1,i} = (k_1/m)Z_{i+1,i}\Delta T$ so that the conductance is $K = (k_1/m)Z_{i+1,i} = -(k_1/m)\varphi_1$, leading us to follow expression for the conductance

$$K = \frac{k_1^2}{2m^2k_0\gamma A_1^2}(mk_B + 2C_1). \quad (36)$$

In this formula the value of C_1 is

$$C_1 = -\frac{1}{2}\frac{dA_1}{dT}y_{11}^e + \frac{\hbar}{4}\frac{dB_1}{dT}, \quad (37)$$

Using formula (5), we obtain explicit expression for A_1 and B_1 , which for $k_1 = 0$ reads

$$A_1 = \frac{\sinh \beta \hbar \omega}{\beta \hbar \omega}, \quad B_1 = \frac{m(\cosh \beta \hbar \omega - 1)}{\beta \hbar}, \quad (38)$$

where $\omega = \sqrt{k_0/m}$. When $k_1 = 0$, $y_{11}^e = mE$ where

$$E = \hbar \omega \left(\frac{1}{e^{\beta \hbar \omega} - 1} + \frac{1}{2} \right). \quad (39)$$

A straightforward algebra leads us to the result

$$K = \frac{K_0}{A_1 k_B} \frac{dE}{dT}, \quad K_0 = k_B \frac{k_1^2}{2m\gamma k_0}. \quad (40)$$

In the classical limit, $E = k_B T$ and $A_1 = 1$ so that $K = K_0$. Thus K_0 is the classical conductance, a result

obtained by Rieder, Lebowitz, and Lieb [1], in the regime of small k_1 . An explicit form for K is

$$K = \frac{K_0(\beta \hbar \omega)^3}{2 \sinh \beta \hbar \omega (\cosh \beta \hbar \omega - 1)}. \quad (41)$$

As regards the behavior with temperature, this result is qualitatively similar to the ones obtained by other approaches [31, 34, 36]. At high temperatures all these approaches give the classical conductance obtained in reference [1], and vanish when $T \rightarrow 0$. However, the behavior at low temperature is distinct. Our results give the behavior $\beta^3 e^{-2\beta \hbar \omega}$ for the conductance whereas the reference [31], for instance, gives the behavior $\beta^{1/2} e^{-\beta \hbar \omega}$.

In conclusion, we have used a quantum FPK equation to cond the contact of a chain of coupled quantum harmonic oscillators with heat reservoirs at distinct temperatures. Starting from the quantum FPK equation, we have set up evolution equations for the covariances and solved them in the stationary regime to get the thermal conductance. An exact closed form for the conductance was obtained for small values of the interparticle interacting parameter. The conductance was found to be finite regardless of the chain length, implying an infinite conductivity and thus the absence of Fourier's law. This is a consequence of the ballistic motion of phonons that occurs in a system with harmonic interactions where the phonons do not interact.

The quantum FPK equation we use holds two important properties with relevant consequences to our analysis. In equilibrium, that is, when the heat baths have the same temperatures, its stationary state is the Gibbs state. Second, it is a canonical quantization of the ordinary FPK equation [25] and, as a consequence it turns into this equation, in the classical limit. Thus, in the classical limit our approach becomes identical to that of Rieder, Lebowitz, and Lieb [1]. We remark that our quantum approach differs from other approaches used to study the thermal transport such as the use of quantum Langevin equations with dissipation proportional to velocity or the use of Lindblad dissipators. Although the quantum FPK equation we used here has not been derived from a full quantum system that includes the reservoirs, we think that the canonical quantization might give support for the validity of the quantum FPK equation, although this procedure does not give an unambiguous prescription for obtaining a quantum version of a classical equation [25]. The present calculation of the conductance, on the other hand, might give indirectly the desired support if we understand that the conductance obtained here is a reasonable result.

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